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Letter to the Editor

High-order zero-dissipative Runge–Kutta–Nyström methods

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Abstract

A new Runge–Kutta–Nyström pair of orders eight and six is presented here. Its main advantage is that it is of zero dissipation so it possesses an interval of periodicity. Numerical results over a set of problems demonstrate the superiority of the method in problems with periodic solution. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

The initial value problem

$$y'' = f(x,y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y_0',$$

where $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$, and $(y_0, y_0') \in \mathbb{R}^{2m}$, is usually approximated at a discrete set of points (x_n, y_n, y_n') by an explicit Runge–Kutta–Nyström (RKN) pair of orders $p(q)$, $p>q$. The form of this method is

$$f_i = f\left(x_n + c_i h_n, y_n + c_i h_n y_n' + h_n^2 \sum_{j=1}^{s} a_{ij} f_j\right), \quad i = 1,2,\dots,s,$$

$$y_{n+1} = y_n + h_n y_n' + h_n^2 \sum_{i=1}^{s} b_i f_i, \qquad \widehat{y}_{n+1} = y_n + h_n y_n' + h_n^2 \sum_{i=1}^{s} \widehat{b}_i f_i,$$

$$y_{n+1}' = y_n' + h_n \sum_{i=1}^{s} b_i' f_i, \qquad \widehat{y}_{n+1}' = y_n' + h_n \sum_{i=1}^{s} \widehat{b}_i' f_i,$$

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with $h_n = x_{n+1} - x_n$, and s the number of the stages of the method. It is assumed that y_n, y'_n are the higher-order approximations which are also used to propagate the solution. Some norm of the vector estimating the error $e = (h_n^2 \sum_{i=1}^{s} (b_i - \widehat{b}_i) f_i, h_n \sum_{i=1}^{s} (b'_i - \widehat{b}'_i) f_i)$, is used in comparison with the requested tolerance TOL, for step-size control.

All the coefficients can be formulated using the Butcher tableau [1]. So the method takes the form

$$\begin{array}{c|c} c & A \\ \hline & b\,\widehat{b} \\ & b'\,\widehat{b}' \end{array}$$

with $A \in \mathbb{R}^{s\times s}, b^{\mathrm{T}}, \widehat{b}^{\mathrm{T}}, b'^{T}, \widehat{b}^{\mathrm{T}}, c \in \mathbb{R}^s$.

In order to test the performance of these methods for periodic problems it is of interest to consider the problem

$$y'' = -\lambda^2 y, \qquad y(0) = 1, \qquad y'(0) = \mathrm{i}\lambda, \quad \lambda \in \mathbb{R}, \tag{1}$$

whose exact solution is $y(x) = \exp(\mathrm{i}\lambda x)$. Application of the RKN method to problem (1) yields the following recursive relation:

$$\begin{bmatrix} y_{n+1} \\ h_{n+1} y'_{n+1} \end{bmatrix} = R(z_n) \cdot \begin{bmatrix} y_n \\ h_n y'_n \end{bmatrix},$$

where $z_n = -H_n^2$, $H_n = \lambda h_n$ and [1]

$$R(z_n) = \begin{bmatrix} 1 + z_n b(I - z_n A)^{-1} e & 1 + z_n b(I - z_n A)^{-1} c \\ z_n b'(I - z_n A)^{-1} e & 1 + z_n b'(I - z_n A)^{-1} c \end{bmatrix}. \tag{2}$$

Following Van der Houwen and Sommeijer [14] we shall say that a RKN method has a zero dissipation if $\det(R(z)) \equiv 1$. This is also essential for a method to possess an interval of periodicity, which is defined to be the interval $(0, z_0)$, for which $-2 < \mathrm{trace}(R(z)) < 2$ for all $0 < z < z_0$.

It is also useful to write Eq. (2) in the form

$$R(z) = \begin{bmatrix} \sum_{i=0}^{\infty} s_{2i-1} z^i & \sum_{i=0}^{\infty} s_{2i} z^i \\ \sum_{i=0}^{\infty} s'_{2i-1} z^i & \sum_{i=0}^{\infty} s'_{2i} z^i \end{bmatrix}$$

with $s_{2i-1} = bA^{i-1}e$, $s_{2i} = bA^{i-1}c$, $s'_{2i-1} = b'A^{i-1}e$, $s'_{2i} = b'A^{i-1}c$, and $s'_{-1} = 0$, $s_0 = s_{-1} = s'_0 = 1$. Then $\det(R(z)) = P \equiv 1 + \sum_{i=0}^{\infty} \widetilde{s}_i z^i$, and $\widetilde{s}_i = 0$ are evaluated with respect to various s, s'. For an explicit RKN method there is an index $i = s$, such that $\widetilde{s}_j = s_j = s'_j = 0$, for all $j \geqslant i$. On the other hand, for a second-order method $s_1 = \frac{1}{2}$, $s'_1 = 1$, $s'_2 = \frac{1}{2}$, etc. Practically a small number of equations for satisfying zero dissipation remains to be solved.

[1] $e = [1, 1, \ldots, 1]^{\mathrm{T}} \in \mathbb{R}^s$.

Table 1
Coefficients of NEW8(6) with zero dissipation (Rational approximations accurate to 18 significant digits)

0									
$\frac{53520637}{572121662}$	$\frac{2232527}{510224080}$								
$\frac{357248860}{1909448607}$	$\frac{2232527}{382668060}$	$\frac{37081334}{3177977723}$							
$\frac{59418235}{171833923}$	$\frac{30566341}{1760496148}$	$\frac{8218085}{734916954}$	$\frac{20946667}{670502569}$						
$\frac{504173341}{1087994762}$	$\frac{8338478}{576439607}$	$\frac{261273394}{6072168265}$	$\frac{29462594}{997634791}$	$\frac{77204245}{3795243917}$					
$\frac{387843305}{481838798}$	$\frac{1100589730}{2256756531}$	$-\frac{2504085737}{1611855801}$	$\frac{7903856905}{4158249776}$	$-\frac{2746138419}{2848012111}$	$\frac{131209591}{289472778}$				
$\frac{862622967}{973409174}$	$-\frac{5574225260}{1895534583}$	$\frac{18077935161}{1758392437}$	$-\frac{9350911807}{861383162}$	$\frac{1948485627}{355652546}$	$-\frac{736004998}{452939571}$	$\frac{30627356}{562404525}$			
1	$\frac{1325770706}{1152764413}$	$-\frac{4839505982}{1296410665}$	$\frac{3190857006}{755292433}$	$-\frac{4573493832}{2249363015}$	$\frac{1400717651}{1651772814}$	$\frac{12114323}{331609812}$	$\frac{3175573}{456323904}$		
1	$\frac{13093931}{251590199}$	0	$\frac{453730323}{1723073015}$	$-\frac{174729768}{1541576453}$	$\frac{154302939}{629373676}$	$\frac{89112923}{1899373863}$	$\frac{3795253}{644583773}$	0	
b	$\frac{13093931}{251590199}$	0	$\frac{453730323}{1723073015}$	$-\frac{174729768}{1541576453}$	$\frac{154302939}{629373676}$	$\frac{89112923}{1899373863}$	$\frac{3795253}{644583773}$		
b'	$\frac{13093931}{251590199}$	0	$\frac{236119875}{728916961}$	$-\frac{145423380}{839364157}$	$\frac{56276012}{123171693}$	$\frac{168458860}{700436693}$	$\frac{36197530}{699693487}$	$\frac{49704941}{1032349655}$	
$\widehat{b}$	$\frac{106709197}{1949525980}$	0	$\frac{189148257}{765523804}$	$-\frac{85259905}{1101513319}$	$\frac{281276824}{1286133115}$	$\frac{25824341}{461156990}$	$\frac{968741}{1095289242}$		
$\widehat{b}'$	$\frac{106709197}{1949525980}$	0	$\frac{463818847}{1525964332}$	$-\frac{379038881}{3203661980}$	$\frac{461048333}{1131231912}$	$\frac{203285488}{708159667}$	$\frac{10565889}{1359619685}$	$-\frac{146565653}{1579900056}$	$\frac{3}{20}$

2. The new method

Unfortunately until now none has constructed RKN of high order with zero dissipation. Actually the higher-order explicit RKN method of zero dissipation is only of fourth order [2]. Even recently [8], much effort was put in order to construct a nondissipative method of the same order. This is probably due to the large number of order conditions for a RKN pair that have to be solved in combination with the zero dissipation conditions. For an 8(6) pair we need to solve 80 nonlinear equations.

Twenty-two equations are needed for y, 37 for y', 8 for $\widehat{y}$ and 13 for $\widehat{y}'$. If we choose $s = 9$ then we produce 80 parameters, and if we were very lucky we could solve the equations. Probably we would admit $s = 10$. But this is not a way to produce a RKN. Here we are going to construct an RKN pair of orders 8(6) that belongs to the Dormand, El-Mikkawy and Prince family [3]. This family requires $s = 9$, but it also uses first stage as last (FSAL) devise, so only eight stages are computed at every step.

Sufficient degrees of freedom are available for the considered RKN implementation, so in companion with equations of condition we can include four equations for satisfying $P \equiv 1$. Setting $\widehat{b}_9 = 3/20$, as in [3], we manage to solve all the above equations and found the nondissipative method given in Table 1.

The interval of periodicity for the new method is a somewhat long one, since $(0, z_0) = (0, 6.13)$. The Euclidean norm for the truncation errors of this method are $\|\tau^{(9)}\|_2 = 2.5 \cdot 10^{-6}$ and $\|\tau'^{(9)}\|_2 = 2.6 \cdot 10^{-6}$, while for DEP8(6) presented in [3] we get $\|\tau^{(9)}\|_2 = 8.3 \cdot 10^{-7}$ and $\|\tau'^{(9)}\|_2 = 8.2 \cdot 10^{-7}$. It is known that the later method possess an empty interval of periodicity.

3. Numerical results

The new method and its main competitor DEP8(6), [3] were tested in some test problems known in the literature of differential equations with periodic solutions. Actually, the selection was done among problems where P-stable methods or even methods with nonvanishing interval of periodicity seems to perform better [10]. In addition, the new type of step control policy for pairs of orders $p(p-\beta)$, $\beta > 1$, introduced in [13], was used here.

(1) The Stiefel and Bettis problem [11],

$$u'' + u = 0.001\cos(x), \qquad u(0) = 1, \qquad u'(0) = 0,$$

$$v'' + v = 0.001\sin(x), \qquad v(0) = 0, \qquad v'(0) = 0.9995.$$

The value $\sqrt{u^2(x) + v^2(x)} - \sqrt{1 + (0.0005x)^2}$ was recorded at the end point $x = 40\pi$.

(2) The problem of Lambert and Watson [5],

$$y_1'' + \lambda^2 y_1 = f''(x) + \lambda^2 f(x), \qquad y_1(0) = \alpha + f(0), \qquad y_1'(0) = f'(0),$$

$$y_2'' + \lambda^2 y_2 = f''(x) + \lambda^2 f(x), \qquad y_1(0) = f(0), \qquad y_1'(0) = \lambda\alpha + f'(0)$$

with $f(x) = \mathrm{e}^{-x/20}$, $0 \leqslant x \leqslant 20\pi$, and theoretical solution $y_1(x) = \alpha\cos(\lambda x) + f(x)$, $y_2(x) = \alpha\sin(\lambda x) + f(x)$. The case $\alpha = 1$, $\lambda = 20$ was the one chosen here.

(3) A Nonlinear example [4],

$$z'' = -(1 + \gamma + \gamma\delta \mathrm{e}^{-2\mathrm{i}x})z + \gamma \mathrm{e}^{-\mathrm{i}x} z^2,$$

$$z(0) = 1 + \delta, \qquad z'(0) = i(1 - \delta),$$

with exact solution the ellipse $z(x) = \mathrm{e}^{\mathrm{i}x} + \delta \mathrm{e}^{-\mathrm{i}x}$. In this problem γ is the nonlinearity parameter and δ is the distortion parameter. So we implemented here the case $\gamma = 0.1$, $\delta = \frac{1}{2}$ and $x \in [0, 20\pi]$.

Table 2
NEW8(6) against DEP8(6)

log global error	Stiefel & Bettis	Non Linear	Lambert & Watson	
−2				
−3			35	
−4			34	
−5		9	36	
−6	73	23	37	
−7	76	22	38	
−8	78	21		
−9	78	8		
−10	80	12		
	77	16	36	43

Efficiency gains tables. Unity represents 1%. Numbers have been rounded to the nearest digit. Positive numbers mean that the first method is superior. The final row, gives the mean value of efficiency gain for all tolerances in a problem. The right most lower number is the average efficiency gain for all problems. Empty places in the tables are due to the unavailability of data for the respective tolerances. See [6] for more details.

The problems were applied for $\mathrm{TOL} = 10^{-3}, 10^{-4}, \ldots, 10^{-9}$. We present the results in Table 2. These results were obtained according to the guidelines given in [9, 6, 12, 13] or even [7]. So, we notify the percentage difference in the number of function evaluations required for achieving a given end-point global error for each problem. We finally observe that the new method is in average 40% more efficient than the conventional one, for the chosen set of periodic problems. The difference for methods of the same order is by no means remarkable.

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